PART 4

LM2-TOXIC

Chapter 7. LM2-Toxic Sensitivity Analysis

Sensitivity analysis is a very efficient tool that can semi-quantitatively demonstrate the uncertainties in the outputs from a water quality model. These uncertainties in the model outputs could result from the uncertainties associated with the forcing time functions; the water and sediment transport; the numerical algorithms used in the model; or the parameters for the chemical and biochemical processes defined in the model. This chapter summarizes the results of a series of sensitivity analyses completed only for the forcing time functions such as primary production and polychlorinated biphenyl (PCB) loads. The PCB atmospheric components (PCB vapor concentration, dry and wet deposition) and tributary PCB load half-lives are discussed in Part 4, Chapters 3 and 6. Model sensitivity analyses were performed over both a short-term (two years, 1994-1995) and long-term (62 years - 1994 to 2055) periods.

4.7.1 Primary Production Sensitivity

Due to the affinity of PCBs for organic carbon, the internal organic carbon load (primary production) is very important in understanding the transport and fate of PCBs in the Lake Michigan system. The internal organic carbon load used in the LM2-Toxic was generated by the eutrophication model, LM3-Eutro (See Part 2 for details). Because there are uncertainties associated with the LM3-Eutro generated internal organic carbon load, the variations in the load on the LM2-Toxic PCB model output concentrations (including solids - dissolved organic carbon (DOC), biotic carbon (BIC), particulate detrital carbon (PDC), and PCBs) were explored. The results of the sensitivity analysis for PCBs are illustrated with the PCB_{28+31} congener pair because it is the most abundant PCB congener pair in Lake Michigan. In LM2-Toxic, this congener pair is modeled as a single state variable. The internal organic carbon load generated from the LM3-Eutro for the LMMBP period (1994-1995) was increased 50% for one analysis and decreased 50% for a second analysis. The model simulations for the analyses were conducted for both a short-term (two-year period: 1994 and 1995) period and a long-term (62-year period: 1994-2055) periods. The results from the sensitivity analysis were compared to the results from the LM2-Toxic model base runs (i.e., calibration run for the 1994-1995 period and long-term Constant Condition Scenario, see Part 4, Chapters 4 and 6 for detailed descriptions of both of these base runs).

Below is a summary of the results from the sensitivity analysis:

1. As shown in Figures 4.7.1 and 4.7.2, a 50% increase or decrease in the primary production has a noticeable effect on the solid concentrations (DOC, BIC, PDC) in the water column compared to the base run concentrations for both short-term and long-term simulations. Table 4.7.1 lists annual average concentrations for the water column carbon solids and the percentage change of the water column carbon solids concentrations due to the increase and decrease in the primary production for both short-term and long-term simulations. Primary production has significant and almost instant

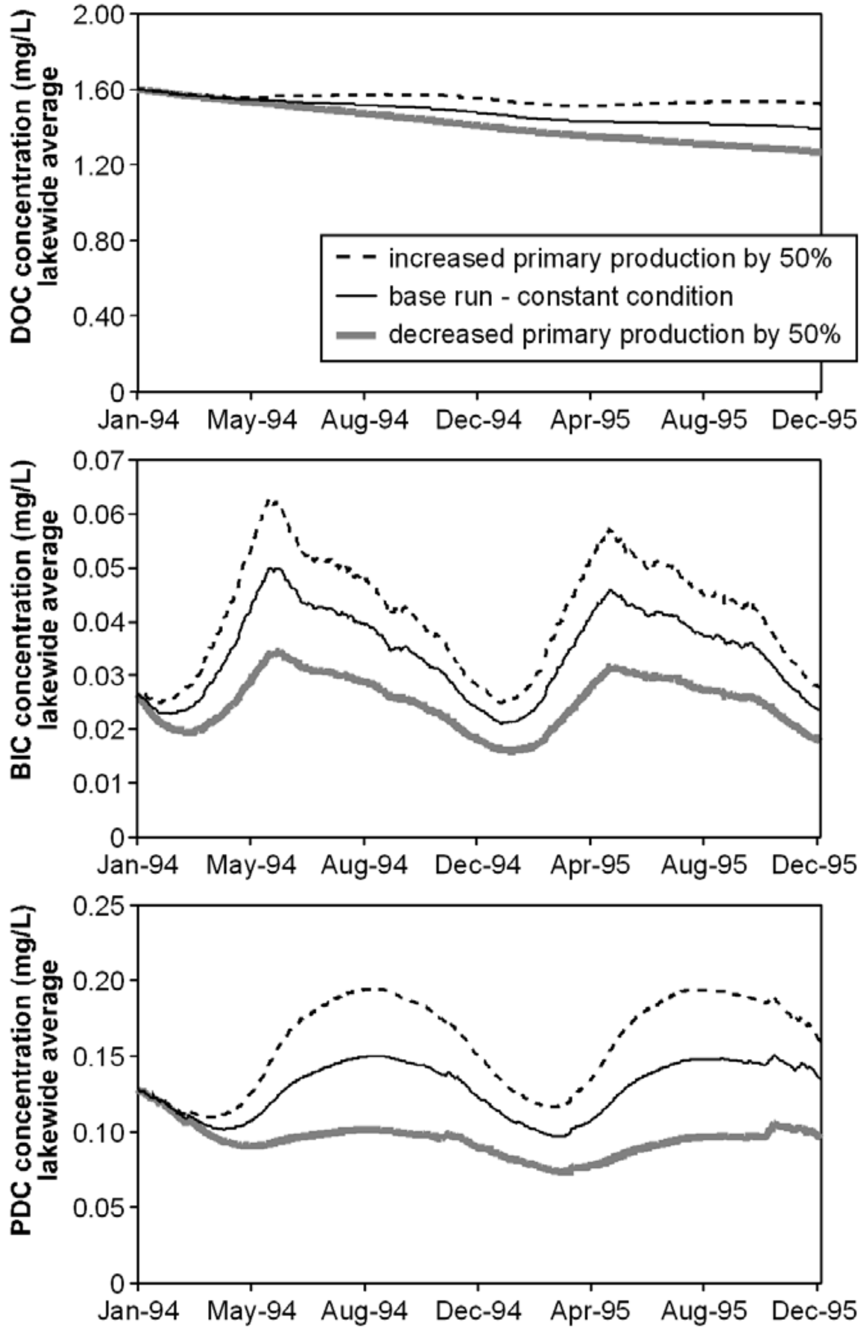

Figure 4.7.1. Short-term (1994-1995) variations of lake-wide (Green Bay included) organic carbon concentrations for ± 50% primary production changes without adjusting settling and resuspension rates.

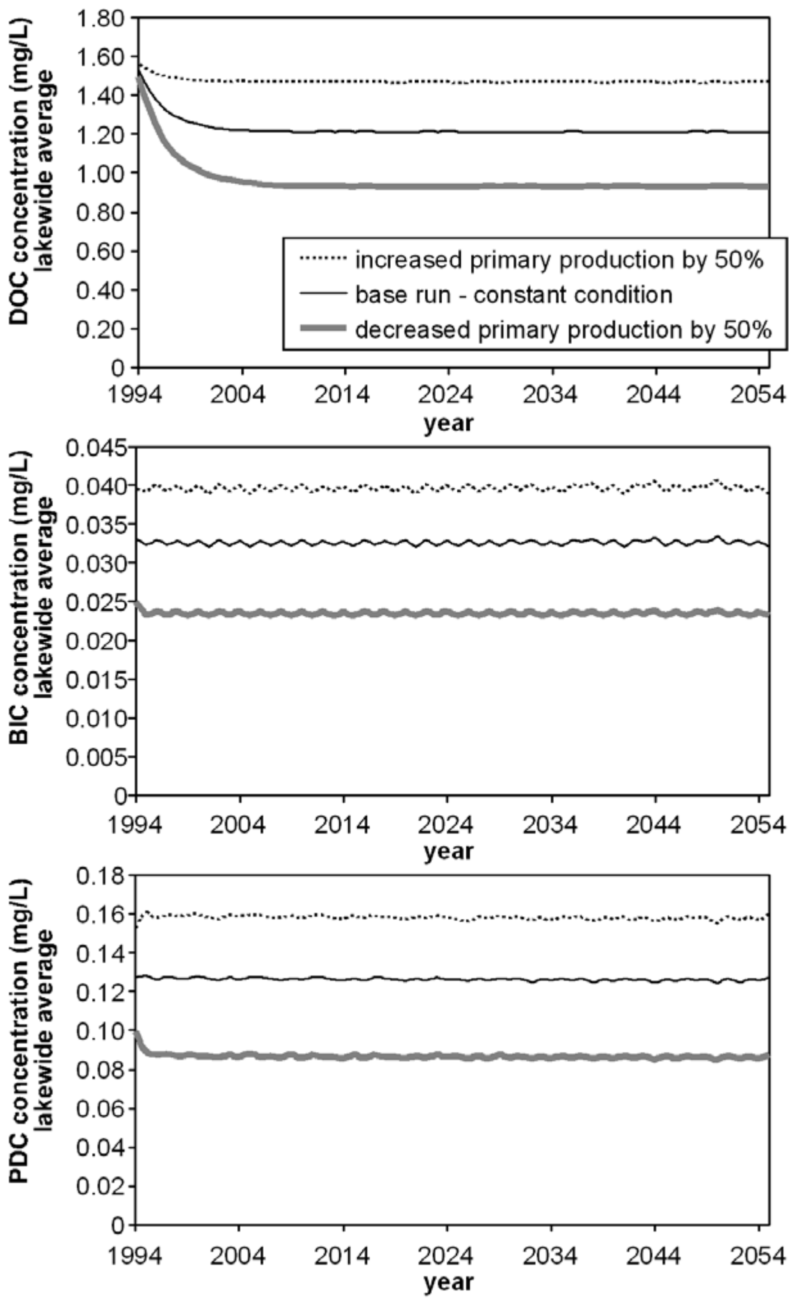

Figure 4.7.2. Long-term (1994-2055) variations of lake-wide (Green Bay included) organic carbon concentrations for ± 50% primary production changes without adjusting settling and resuspension rates.

Table 4.7.1. Annual Average Concentrations of Water Column Carbon Solids and Annual Average Change in Percentage for Water Column Carbon Solids Concentrations Resulting From the LM2-Toxic Model Runs for Both the Short-Term (1994-1995) and the Long-Term (1994-2055) Simulations With 50% Increase and 50% Decrease of the LM3-Eutro Produced Primary Production

Carbon Solids (Short-Term Simulations)	Concentration (mg/L) From Original Base	Concentration (mg/L) From the Run With 50% Reduction	Annual Average Percentage (%) Change	Concentration (mg/L) From the Run With 50% Increase	Annual Average Percentage (%) Change
DOC	1.48	1.42	-4	1.55	5
BIC	0.034	0.025	-27	0.042	23
PDC	0.129	0.095	-26	0.159	23
Carbon Solids (Long-Term Simulations)					
DOC	1.23	0.96	-22	1.47	20
BIC	0.034	0.025	-27	0.042	23
PDC	0.129	0.088	-32	0.162	26

impact on the level of BIC and PDC concentration in the water column. Because of much larger initial DOC inventory in the lake and slower degradation process from PDC to DOC, the impact on DOC concentration in the lake due to the changes of primary production was not as evident as on BIC and PDC in the early portion of the long-term simulation period.

2. Figure 4.7.3 shows that, compared with the base run, there is very little difference in the PCB water column concentrations generated from the runs with 50% decrease and a 50% increase in primary production for the short-term simulation. Table 4.7.2 provides detailed information on individual mass fluxes in Lake Michigan and PCB inventories of both water column and surficial sediment for the two-year (1994-1995) sensitivity analyses. The decrease and increase in the settling PCB mass flux due to the 50% decrease and the 50% increase in primary production were compensated by the increase and decrease in the gross volatilization mass flux, respectively. This keeps the PCB water column inventories predicted from these two runs very close to the inventory generated from the short-term base runs.

3. The long-term, steady-state PCB concentrations in the water column was not significantly different from the base run concentrations (Figure 4.7.4). Interestingly, PCB concentrations from the long-term sensitivity runs started out almost identical and deviated with each other toward the end of the simulation. Table 4.7.3 provides detailed information on individual PCB mass fluxes in Lake Michigan and inventories of both the water column and the surficial sediment for the last two years of the long-term (62-years) model simulation. Similar to the short-term simulation, PCB settling and net volatilization fluxes were affected the most by the increase and the decrease of the primary production. The increase or decrease of the settling fluxes due to the increase or decrease in primary production was countered by the decrease or increase of the net volatilization fluxes.

In conclusion, the sensitivity analyses illustrate that, under the 1994-1995 PCB loading/boundary conditions/other forcing functions, a 50% increase or decrease in primary production generated from the LM3-Eutro does not have a significant influence on PCB concentrations in Lake Michigan for both short-

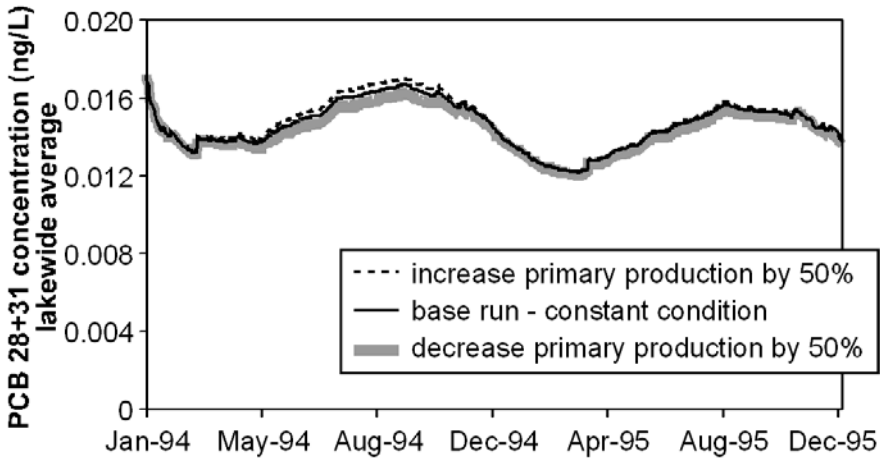

Figure 4.7.3. Short-term (1994-1995) variations of lake-wide (Green Bay included) PCB_{28+31} (dissolved + particulate) concentrations for ± 50% primary production changes without adjusting settling and resuspension rates.

Table 4.7.2. PCB_{28+31} Mass Fluxes and Inventories for Lake Michigan System Results From the LM2-Toxic Sensitivity Analysis on Primary Production for the Short-Term (Two-Year Period: 1994-1995) Simulations

PCB Mass Fluxes, kg/(Two Years) and Inventories, kg	Original Base Run	50% Reduction	50% Increase
Loads	113.97	113.97	113.97
Settling	104.62	89.58	116.06
Resuspension	175.59	176.77	170.48
Burial	135.99	134.12	137.80
Water Column Inventory	70.79	69.67	71.41
Sediment Inventory	808.76	797.63	819.53
Diffusion	33.37	34.20	32.73
Absorption	265.30	265.30	265.30
Gross Volatilization	558.01	577.43	540.79
Net Volatilization	292.71	312.13	275.49
Export to Lake Huron	0.88	0.78	0.97
Chicago Diversion	0.09	0.08	0.09
Mass Gain/Loss in Water Column	-75.38	-77.64	-75.43

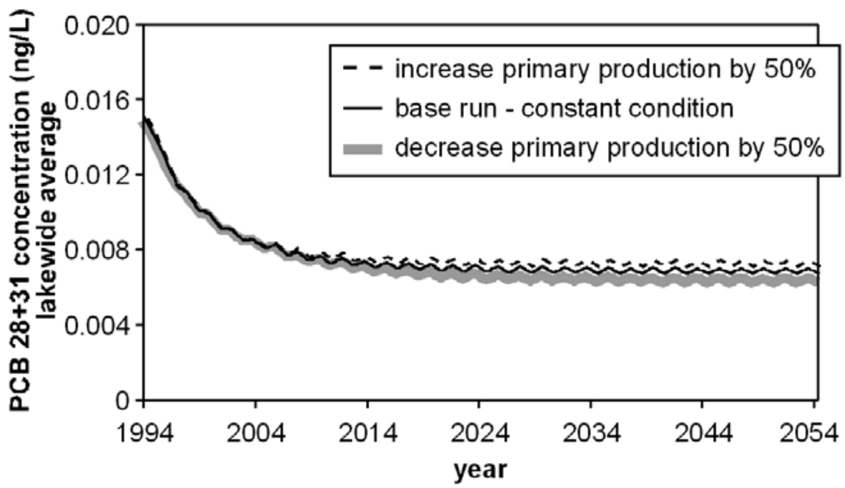

Figure 4.7.4. Long-term (1994-2055) variations of lake-wide (Green Bay included) PCB_{28+31} (dissolved + particulate) concentrations for ± 50% primary production changes without adjusting settling and resuspension rates.

Table 4.7.3. PCB_{28+31} Mass Fluxes and Inventories for Lake Michigan System Results From the LM2-Toxic Sensitivity Analysis on Primary Production For the Last Two Years of the Long-Term (62-Year Period: 1994-2055) Simulations

PCB Mass Fluxes, kg/(Two Years) and Inventories, kg	Original Base Run	50% Reduction	50% Increase
Loads	113.97	113.97	113.97
Settling	43.80	32.47	51.94
Resuspension	25.17	23.42	24.68
Burial	21.98	22.39	21.81
Water Column Inventory	33.78	31.21	35.71
Sediment Inventory	130.74	133.13	129.71
Diffusion	0.52	0.70	0.46
Absorption	263.07	263.07	263.07
Gross Volatilization	355.33	365.30	346.47
Net Volatilization	92.26	102.23	83.40
Export to Lake Huron	0.69	0.58	0.77
Chicago Diversion	0.07	0.06	0.07
Mass Gain/Loss in Water Column	2.84	2.73	2.93

term and long-term forecast scenarios. Table 4.7.4 lists the model-generated average PCB inventories resulting from the sensitivity runs for both the water column and the surficial sediment layer and the percentage change of the average PCB inventories in both compartments due to the increase and decrease in primary production. The inventories are the average PCB inventories for the two-year period of the short-term (1994-1995) simulation and the last two-year period of the long-term simulation. The largest percentage change of PCB inventories due to the 50% increase or decrease in primary production goes to the PCB inventory in the water column at the end of the long-term simulation period and is in the range of 5-8%. The impact on PCB inventory of the surficial sediment layer due to the changes of primary production is very small for both the short-term and the long-term periods.

4.7.2 PCB Loads Sensitivity

The variation in the outcomes of PCB concentrations in both the water column and sediment from the LM2-Toxic model can be very significant due to the uncertainty of PCB loads used as input. The uncertainty of the LMMBP-generated PCB loads could be due to sampling approach, analytical method, interpolation algorithm used for estimating the loads, and loads that were missed or not considered.

There is evidence (Wethington and Hornbuckle, 2005) that an additional input of PCBs was contributed from the local Milwaukee atmosphere through vapor-water exchange and wet and dry deposition to Lake Michigan that were not accounted for in the LM2-Toxic model. The combined additional PCB source from the Milwaukee regional atmosphere was estimated to be at least 120 kg per year (Wethington and Hornbuckle, 2005). It is possible that loads in other areas of the basin could have been missed, such as Green Bay.

Another potential unaccounted PCB source to the lake is the load associated with very large atmospheric particles. These are particles with a diameter greater than 10 µm and settling velocities greater than 7.4 cm s^{-1}. Although there is some disagreement among experts in the field regarding the magnitude of PCB loads to the lake *via* the large particles, studies indicate that PCB dry deposition associated with large particles could be a significant PCB source to the lake (Miller *et al*., 2001; Franz *et al*., 1998; Holsen *et al*., 1991). The annual PCB inputs from the atmosphere through the coarse particles could be in a range of 320 kg/year to 5,500 kg/year (data provided from the LMMBP atmospheric working group; Wethington and Hornbuckle, 2005; Franz *et al*., 1998; and Holsen *et al*. 1991) during the period of 1989-1995. However, the science and technique is not well-developed enough to make reliable over-lake estimates of these fluxes. Much of the uncertainty in measuring large particle fluxes comes from the difficulty in quantifying how far these large particles travel from their source to the lake.

Model runs were designed to evaluate the impact of potential missing loads on the model outputs. A sensitivity analysis was completed for the Milwaukee load by adding 120 kg/year of PCB load into segment 1 in the LM2-Toxic model. Additional simulations were run to gain insight into how the model would respond to increasing the total PCB load (tributary load + atmospheric load) by 50% and 100%. The results from the sensitivity analysis were then compared with the LM2-Toxic model long-term (62 years) base run results (Figure 4.7.5). Compared to the steady-state concentration from the long-term base run, the simulation showed total PCBs in the water column increased less than 5% for the suggested 120 kg/year missing PCB source from the Milwaukee atmosphere. An increase of 15% and 30% was found for the simulations where the PCB load was increased by 50% and 100%, respectively. The amount of increase in total PCB concentrations was much less during the first five years of the simulation than during the steady-state period. This indicates that, under the current conditions in the Lake Michigan system, the LMMBP-generated PCB loads were not the dominant PCB flux controlling the concentration of PCBs in the lake. When the load was doubled, the PCB concentrations in the water column in the first few years only increased about 15%. Part 4, Chapter 6 provides quantitative analyses and in-depth discussions on the critical sources and sinks and important environmental processes for PCBs in Lake Michigan.

Table 4.7.4. PCB_{28+31} Average Inventories of Water Column and Surficial Sediment Results From the LM2-Toxic Simulations for the Primary Production Sensitivity Analysis, and Changes in Percentage for These Inventories Compared to the Inventories From the Original Base Runs

PCBs (Short-Term Simulations)	Inventory (kg) From the Original Base Run	Inventory (kg) From the Run With 50% Reduction in Primary Production	Percent (%) Change	Inventory (kg) From the Run With 50% Increase in Primary Production	Percentage (%) Change
Water Column	70.79	69.67	-1.6	71.41	0.88
Surficial Sediment	808.76	797.63	-1.4	819.53	1.3
PCBs (Long-Term Simulations)					
Water Column	33.78	31.21	-7.6	35.71	5.7
Surficial Sediment	130.74	133.13	1.8	129.71	-0.79

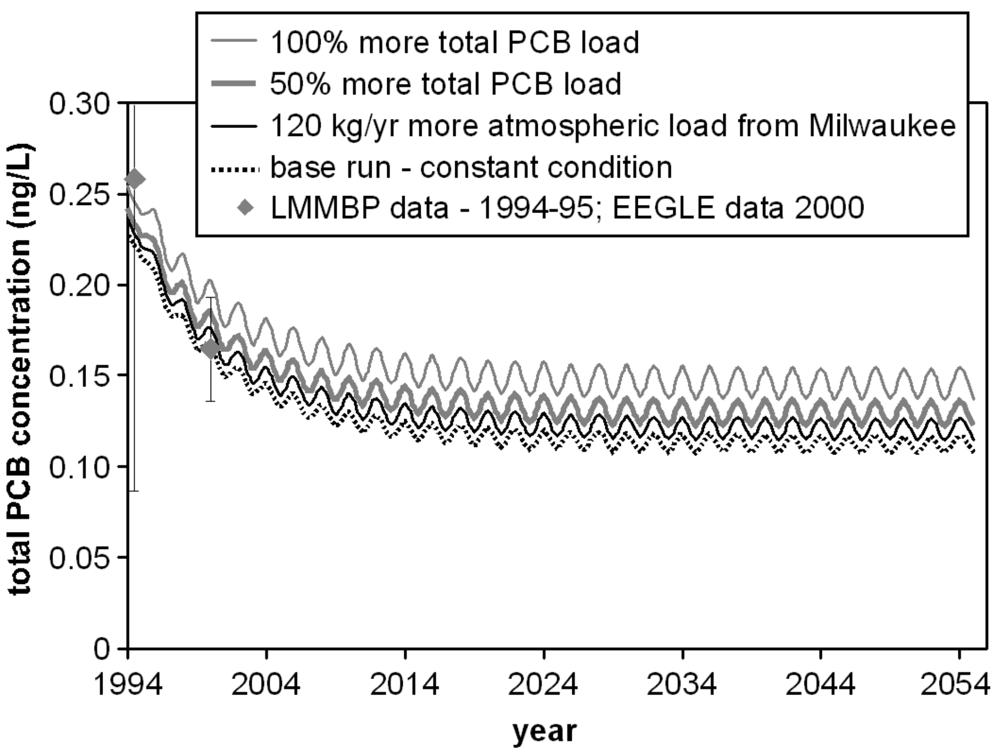

Figure 4.7.5. Sensitivity analysis of the LM2-Toxic predictions to varying PCB loads. Note: LMMBP data - 1994-1995 = 0.259 ± 0.172 ng/L; EEGLE data 2000 = 0.165 ± 0.029 ng/L. The model output concentrations and field data in this graph are lake-wide average concentrations.

References

Franz, T.P., S.J. Eisenreich, and T.M. Holsen. 1998. Dry Deposition of Particulate Polychlorinated Biphenyls and Polycyclic Aromatic Hydrocarbons to Lake Michigan. Environ. Sci. Technol., 32(23):3681-3688.

Holsen, T.M., K.E. Noll, S. Liu, and W. Lee. 1991. Dry Deposition of Polychlorinated Biphenyls in Urban Areas. Environ. Sci. Technol., 25(6):1075-1081.

Miller, S.M., M.L. Green, J.V. DePinto, and K.C. Hornbuckle. 2001. Results From the Lake Michigan Mass Balance Study: Concentrations and Fluxes of Atmospheric Polychlorinated Biphenyls and *trans*-Nonachlor. Environ. Sci. Technol., 35(2):278-285.

Wethington, D.M. and K.C. Hornbuckle. 2005. Milwaukee, WI, as a Source of Atmospheric PCBs to Lake Michigan. Environ. Sci. Technol., 39(1):57-63.